Propane, 1,1,3,3-tetramethoxy-
102-52-3 | DTXSID4059255

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.99e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.32e-01

Confidence level: 4.88e-01

Nearest Neighbors from the Training Set

Image not found
2-(2-Ethoxyethoxy)ethyl acetate
Measured: 5.68
Predicted: 7.71e-01

Image not found
2,5-dimethoxy-2,5-dimethyl-1,4-dioxane
Measured: 5.68e-02
Predicted: 2.72e-01

Image not found
Dimethyl adipate
Measured: 3.44e-02
Predicted: 1.69e-01

Image not found
Dimethyl glutarate
Measured: 3.68e-01
Predicted: 4.48e-01